

A HEURISTIC DERIVATION OF THE SCHRÖDINGER EQUATION AND THE MOMENTUM OPERATOR

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ABSTRACT. Students in a quantum mechanics course are often introduced to the Schrödinger equation as the standard mathematical tool. However, rarely do students develop an understanding as to why the equation is the choice for modeling quantum phenomena or where it came from. While many books do have a heuristic derivation, they sometimes differ in their approach and often fail to give a satisfying explanation to the so-called canonical substitution of momentum. In this paper, we use de Broglie's hypothesis along with experimental results and theories to provide a heuristic derivation of the Schrödinger equation and of the momentum operator.

1. INTRODUCTION

The Schrödinger equation is a partial differential equation given by

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V(x) \Psi \quad (1.1)$$

where Ψ satisfies an initial condition $\Psi_0 = \Psi(0, t)$. It was derived as a modeling tool in quantum mechanics by Erwin Schrödinger in 1925-1926, and its fidelity to reality earned him the Nobel Prize. Its wave function (solution) represents the state of a very small particle such as an electron. Particles at such a small size scale exhibit a so-called wave-particle duality. Introductory quantum mechanics books (see for example [9]), typically introduce the Schrödinger equation to the reader, and use it to theoretically arrive at some of the fundamental concepts that show up experimentally. Consequently, some students are left wondering where the equation came from or how Erwin Schrödinger devised it. Indeed many texts and papers give derivations of (1.1). However, most of these are for more advanced students and thus have derivations that are mathematically inclined and do not emphasize the physical motivation (see [10] and [7]).

It is common practice to write (1.1) as

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{\mathbf{p}^2}{2m} \Psi + V \Psi \quad (1.2)$$

where \mathbf{p} is the momentum operator given by the following substitution:

$$\mathbf{p} \longrightarrow -i\hbar \nabla. \quad (1.3)$$

It is evident that this is not the form of momentum that students are used to seeing in classical mechanics. While some sources of the literature do provide a derivation of this canonical substitution, it usually is also very mathematical in nature. Furthermore, most introductory text books in quantum mechanics implore the reader to accept this substitution as standard.

Key words and phrases. Schrödinger equation, quantum mechanics, heuristic derivation, momentum operator, Eigenfunction, eigenstates.

This paper presents a brief heuristic derivation of the Schrödinger equation and the momentum operator in the context of quantum mechanics. The derivation presented follows those derivations of various sources including [9], [10], and [11]. While there is nothing novel in the discussed approach, the paper attempts to present a brief and accessible introduction to the equation that should provide students in an introductory course with a deeper understanding of the Schrödinger equation in quantum mechanics. The main purpose of the paper is thus pedagogical in nature.

Rather than following the path of mathematical formalism, we take a heuristic approach and acquaint the reader with experimental results and the theories of Bohr, Einstein and de Broglie. After this brief review of the physical history of quantum mechanics, we derive a wave equation that satisfies three physically motivated requirements:

- (1) The total energy, E satisfies $E = \frac{p^2}{2m} + V$, where each term is the kinetic and potential energy respectively.
- (2) Our equation should in some way reflect the theories of Einstein and De Broglie.
- (3) The equation must be linear so that solutions may be superimposed.

We shall elaborate on these requirements as we review our quantum mechanical history. We then introduce some of the basic mathematical tools required to study the equation and its implications. We conclude by giving a simple argument for the quantum-mechanical operator. As a result, the reader should develop intuition and a better understanding of the Schrödinger equation and ultimately, of quantum mechanics.

2. HISTORY

At the end of the 19th century, physics was on the verge of great discovery in what would be one of the most important subfields to define modern physics. While the general consensus in the physics community was that there were no more great discoveries left, there were some unsettling experimental results that were not understood. It was then that scientists such as Planck, Bohr, and Einstein ushered in a new era that would help understand these results. Eventually this movement was formalized into a field of modern physics in its own right known as quantum mechanics. Along with the theory of relativity, quantum mechanics seemingly defied logic and intuition. Yet, quantum theory was able to accurately explain the rare occurrences related to very small particles such as electrons and photons. To better understand these occurrences, we will take a journey into the seemingly strange history of the quantum world.

2.1. The Photoelectric Effect and Hydrogen Lights. In 1887, Heinrich Hertz observed the Photoelectric Effect, a phenomena in which electrons are emitted from a sheet of metal upon light absorption. At that time, it was also known that a gaseous atomic hydrogen would glow under some electric discharge. When the emitted hydrogen light would pass through a prism, it would break up into four visible wavelengths of light. In 1888, Johannes Rydberg established a precise mathematical relation between these visible wavelengths (λ) and a pair of integers with a constant R :

$$\frac{1}{\lambda} = R \left(\frac{1}{m^2} - \frac{1}{n^2} \right), \quad m, n \in \mathbb{N}. \quad (2.1)$$

At the dawn of the 20th century Albert Einstein (see [8]) gave an explanation for the photoelectric effect that earned him the Nobel prize (1921). He proposed that the effect was caused by the

absorption of light particles he called photons. His model was based on the work of Max Planck. Essentially, he proposed that the energy of a photon is proportional to the frequency of light:

$$E = hf = \hbar\omega, \quad (2.2)$$

where $\omega = 2\pi f$ and $\hbar = \frac{h}{2\pi}$. In his theory, Einstein proposed that the electrons in the metal sheet required a minimum amount of energy in order to "jump". In the case of light absorption, a photon of energy hf "bumps" into an electron and transfers at most hf energy to the electron. If the minimum required for a jump is exceeded, then the electron has enough energy to be removed from the metal. This minimum, denoted as $\phi = hf_0$, is specifically determined by the specific metal.

2.2. An Atom Model. As discoveries of the Atom and its structure surfaced, models of the Atom were suggested. Ernest Rutherford proposed a planetary model for the atom in which electrons surrounded a positively charged nucleus, much like the planets of the solar system surround the sun in their respective orbits. Unfortunately, according to his planetary model, the Larmor Formula of electrodynamics predicted that in a fraction of a second, electrons would spiral inward and crash into the nucleus. In 1913, Bohr finally proposes the so-called Bohr model in which he mathematically demonstrates that the electron can only occupy certain orbits around the nucleus and can have only certain energies. To understand how he did this we must revisit two important formulas: Coulomb's Law for force between two charged particles and Centripetal Force. Coulomb's Law is a formula in which the force of repulsion between two electric charges, q_1 and q_2 , at a distance r from each other, is given by

$$F = \frac{k_e q_1 q_2}{r^2}, \quad (2.3)$$

where $k_e = \frac{1}{4\pi\epsilon_0}$. The Centripetal Force formula

$$F = \frac{mv^2}{r}, \quad (2.4)$$

gives us the inward-directed force of a particle that is moving at a speed v along a circle of radius r .

The formula for angular momentum is given by $L = pr = mvr$. The key assumption in Bohr's model, was that the angular momentum moment itself must be quantized. Similar to Einstein, Bohr assumed that $L = n\hbar$. It was then easy to show that

$$r_n = n^2 \frac{\hbar^2}{me^2 k_e} = n^2 a_0 \quad (2.5)$$

and

$$E_n = \frac{-k_e e^2}{2n^2 a_0}. \quad (2.6)$$

These results follow from matching the magnitude of the forces given by Centripetal Force (2.4) and Coulomb's Law (2.3).

One of the nice results of the Bohr Model, is that via (2.6), one can theoretically derive the Rydberg formula: If one assumes that each photon in a glowing atom of hydrogen is due to an electron jumping from a higher orbit r_n to a lower orbit r_m , then the energy of the photon is given by

$$E_\gamma = E_n - E_m = hf. \quad (2.7)$$

Since frequency is given by $f = \frac{\text{velocity}}{\lambda}$, we have

$$\frac{1}{\lambda} = \frac{k_e e^2}{2a_0 h c} \left[\frac{1}{m^2} - \frac{1}{n^2} \right], \quad m, n \in \mathbb{N}. \quad (2.8)$$

2.3. De Broglie's Hypothesis. In 1924, Louis de Broglie introduced his hypothesis of the wave-particle duality of matter, based on the work of Albert Einstein and Max Planck with light. In a nutshell, he argued that any particle could be associated with a wave Ψ . He proposed the following relation for the momentum p of the particle and the wavelength λ of its associated wave function:

$$p = \frac{h}{\lambda} = \hbar k, \quad (2.9)$$

where $k = \frac{2\pi}{\lambda}$. This is known as de Broglie's hypothesis.

3. DERIVATION

To understand how to construct the Schrödinger Equation, we must realize that we are simply trying to construct a wave equation. It is not the standard Wave Equation, but an equation that specifically addresses the wave-particle duality of the electron and of the photon. A good example that provides an intuitive understanding of this duality is the famous Double-Slit Experiment. A detector screen is placed at a distance from a light source or an electron gun. Between them, is a plate with two slits. Intuitively, we would expect photons or electrons to behave like discrete particles leaving two distributions on the screen, each with a mode corresponding to the center of each slit. However, when the particles go through the two slits a third distribution is created between the other two expected distributions with no other slit to account for it. This is known as an interference pattern and is characteristic of waves. In constructing our special wave equation, we must therefore have a mathematical superposition principle for our solution so that the interference effect can take place.

We summarize the requirements that our equation must satisfy:

- (1) The total energy, E satisfies $E = \frac{p^2}{2m} + V$, where each term is the kinetic and potential energy respectively.
- (2) We must use (2.2) as the energy of a photon and (2.9).
- (3) The equation must be linear to allow for the superposition principle and the construction of wave packets. In fact, the coefficients of the equation must only have constants so that we can superimpose our solutions over different values of the other parameters, such as frequency.

Since his sought equation should be a wave equation of sorts, it was evident to Erwin Schrödinger that in the case of a free particle ($V = 0$), the wave function should have a trigonometric form or a traveling wave form,

$$\Psi(x, t) = e^{i(kx - \omega t)}. \quad (3.1)$$

By assuming requirement (1) and (2) with $V = 0$, we have that

$$\omega = \frac{\hbar k^2}{2m}. \quad (3.2)$$

Thus, we construct an equation by making sure that requirement (3) is satisfied in a coefficient γ when using (3.1) as a solution. We first try the standard Wave Equation:

$$\frac{\partial^2 \Psi}{\partial t^2} = \gamma \frac{\partial^2 \Psi}{\partial x^2}. \quad (3.3)$$

But this leads to

$$\gamma = \frac{p^2}{4m^2}. \quad (3.4)$$

If instead of (3.3), we try

$$\frac{\partial \Psi}{\partial t} = \gamma \frac{\partial^2 \Psi}{\partial x^2}, \quad (3.5)$$

we find that

$$\gamma = \frac{\hbar i}{2m}. \quad (3.6)$$

Ergo, we obtain the free Schrödinger Equation for the case of the Free Particle:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \quad (3.7)$$

In the case of three dimensions, we simply have $p = \hbar \mathbf{k}$ where \mathbf{k} is a vector in \mathbb{R}^3 such that $|\mathbf{k}| = \frac{2\pi}{\lambda}$. If we add some external force, derivable from a potential V , we would have the general Schrödinger Equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V \Psi \quad (3.8)$$

4. PHYSICAL MEANING

Max Born, suggested that to use the wave function Ψ for physical meaning, one must use $|\Psi|^2$ as a probability density function. Thus, the probability of finding a particle between point a and b on an interval (or space) is given by

$$P(a, b) = \int_b^a |\Psi(x, t)|^2 dx. \quad (4.1)$$

Naturally, the probability of finding the particle anywhere in the in an interval (or space) should be 1:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1. \quad (4.2)$$

The extension to space is done by considering a triple-integral. (4.1) and (4.2) constitute the so-called statistical interpretation.

5. OBSERVABLES

The idea now is that one can use the solution of (1.1) to find averages of physical observables such as position x , or momentum p . In general, we can find expectation values of any physical observable Q , by computing

$$\langle Q \rangle = \langle Q\Psi, \Psi \rangle = \int (Q\Psi) \Psi^* dx. \quad (5.1)$$

It is important that we examine and understand the interpretation of the expectation values of such observables with an example: $\langle x \rangle$ (see [9]). This value is NOT the average of position measurements over the same particle. It is the average of position measurements on different particles all in the same state Ψ . Thus, if we had an ensemble of many different particles all in the same state, and we measure their position at the same time, we will find the average of the position to be $\langle x \rangle$.

5.1. Eigenfunctions, Eigenvalues and the Momentum Operator. We conclude this note by deriving the Momentum operator as an eigenfunction of de Broglie's hypothesis. In essence, we are giving justification for the substitution (1.3), which in 1 dimension can be written as

$$\mathbf{p} = -i\hbar \frac{\partial}{\partial x}. \quad (5.2)$$

Operators can have eigenfunctions with associated eigenvalues. Specifically, f is an eigenfunction of Q if

$$Qf = qf, \quad (5.3)$$

where q is the eigenvalue. For example, to find determinates states of

$$Q = \frac{\hbar}{i} \frac{d}{dx}, \quad (5.4)$$

we solve the following equation

$$\frac{\hbar}{i} \frac{d}{dx} f_p(x) = p f_p(x). \quad (5.5)$$

The general solution is

$$f_p(x) = A \exp\left(\frac{ipx}{\hbar}\right), \quad (5.6)$$

where A is a constant. This is a sinusoidal wave with wavelength

$$\lambda = \frac{2\pi\hbar}{p}. \quad (5.7)$$

We specifically chose p to represent the eigenvalue of (5.4) to remind the reader that (5.7) is de Broglie's hypothesis (equation (2.9)). Thus we can define the momentum operator as (5.2).

REFERENCES

- [1] J.B. Conway, *A Course in Functional Analysis*, second edition, Springer-Verlag, New York, Berlin, Heidelberg, 1990.
- [2] R. Cordero-Soto and S.K. Suslov, *Time reversal for modified oscillators*, Teoret. Mat. Fiz., 2010, **Volume 162**:3, 345-380.
- [3] R. Cordero-Soto, Erwin Suazo and S. K. Suslov, *Models of Damped Oscillators in Quantum Mechanics*, Journal of Physical Mathematics, **1** (2009), S090603.
- [4] R. Cordero-Soto, R. M. Lopez, E. Suazo, and S. K. Suslov, *Propagator of a charged particle with a spin in uniform magnetic and perpendicular electric fields*, Lett. Math. Phys. **84** (2008) #2-3, 159-178.
- [5] M. Meiler, R. Cordero-Soto, and S. K. Suslov, *Solution of the Cauchy problem for a time-dependent Schrodinger equation*, J. Math. Phys. **49** (2008) #7.
- [6] R. Cordero Soto, and M. Engman *Intrinsic Spectral Geometry of the Kerr-Newman Event Horizon*, J. Math. Phys. **47** (2006).
- [7] L. Debnath and P. Mikusiński, *Introduction To Hilbert Spaces with Applications*, third edition, Elsevier Academic Press, Amsterdam, Boston, Heidelberg, 2005.
- [8] A. Einstein, *Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt*, Ann. Phys. **17**(1905), 132-148.
- [9] D.J. Griffiths, *Introduction to Quantum Mechanics*, second edition, Pearson Prentice Hall, Upper Saddle River, New Jersey, 2005.
- [10] S. J. Gustafson and I. M. Sigal, *Mathematical Concepts of Quantum Mechanics*, Springer-Verlag, Berlin, Heidelberg, New York, 2000.
- [11] L.I. Schiff, *Quantum Mechanics*, first edition, McGraw-Hill Book Company, Inc., New York, Toronto, London, 1949.
- [12] <http://www.wikipedia.org/>

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